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Modeling a thermionic energy converter using finite-difference time-domain particle-in-cell simulations

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A thermionic energy converter (TEC) is a static device that converts heat directly into electricity by boiling electrons off a hot emitter surface across a small inter-electrode gap to a cooler collector surface. The main challenge in TECs is overcoming the space charge limit, which limits the current transmitted across a gap of a given voltage and width. We have verified the feasibility of studying and developing a TEC using a bounded finite-difference time-domain particle-in-cell plasma simulation code, OOPD1, developed by Plasma Theory and Simulation Group, formerly at UC Berkeley and now at Michigan State University. In this preliminary work, a TEC has been modeled kinetically using OOPD1, and the accuracy has been verified by comparing with an analytically solvable case, giving good agreement. With further improvement of the code, one will be able to quickly and cheaply analyze space charge effects, and seek designs that mitigate the space charge effect, allowing TECs to become more efficient and cost-effective. © *2014 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4865828]

I. INTRODUCTION

Energy has emerged as one of the biggest challenges facing civilization. Current technology for conversion of heat to electric energy relies on devices containing working fluids or moving parts resulting in lower efficiency due to thermal and friction losses. Furthermore, these existing technologies require maintenance and have limited reliability due to degradation of frictional parts, or fluid characteristics and leakage. High grade heat sources used to drive mechanical conversion systems suffer from losses of 30%–40% due to friction and fluid losses, as well as venting as much as 40% of the energy as waste heat. System complexity and cost are also driven by conversion mechanisms. Direct conversion of part or all of the heat to electrical energy could be part of an overall efficiency improvement strategy. The direct conversion mechanism should not only be efficient but also inexpensive, compact, and low maintenance. Potential applications range from high temperature small engine designs to nuclear power direct converters, in addition to high reliability applications such as satellites.

Thermionic energy converters (TECs) are static energy conversion devices capable of converting heat directly to electricity, using electrons as the working fluid. The first serious investigation of the use of thermionic energy for the generation of electrical power was the work of Hatsopoulos.[1] In his doctorate thesis at MIT in 1956, he described a high vacuum converter having a spacing of a thousandth of an inch and an efficiency of about 13%. The basic TEC is comprised of an emitting and a collecting electrode in vacuum, as shown in Fig. 1(a). The operating principle is based on the thermionic emission of electrons from a hot emitter surface across a small inter-electrode gap to a cooler collector surface, generating a current that can flow back to the cathode through an external load to perform electrical work. TECs have many attractive properties, including high reliability and low weight, and because they are direct thermal-electric conversion, TECs can operate at high temperatures and hence, high Carnot efficiency without suffering losses via friction or in the working fluid.[2,3] Although TECs have been explored for many years and practical systems have been developed and applied in space stations and nuclear plants, etc., TECs today still fall short on the energy conversion efficiency due to physical limiting factors including: (1) Space charge effects, which limit the flow of electrons across the gap, (2) radiation heat transfer between electrodes, and (3) thermal energy losses to the environment. One method of enhancing the efficiency of TECs is overcoming the space charge limitation, which limits the amount of current that can flow across a gap of a given voltage and width.[4,5]

It is not possible to investigate experimentally many of the variables governing the performance of a TEC. Computer simulation is a key tool for understanding the physics of the TEC, leading to improvement of the

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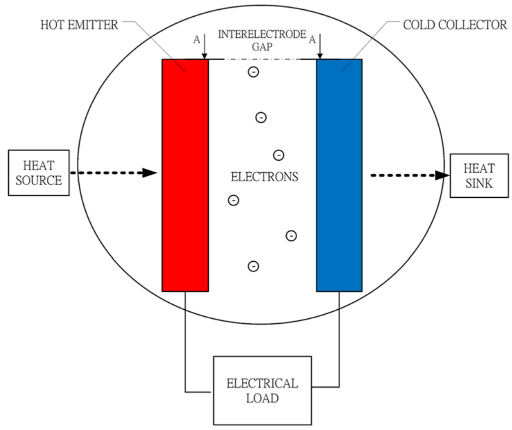
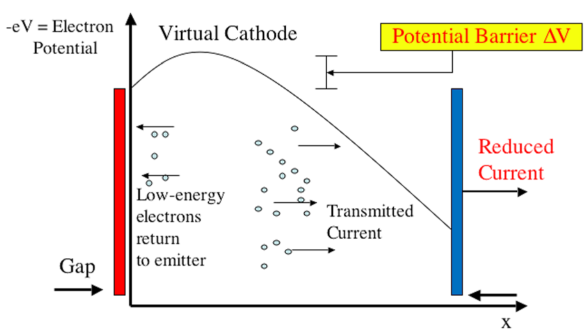


(a)



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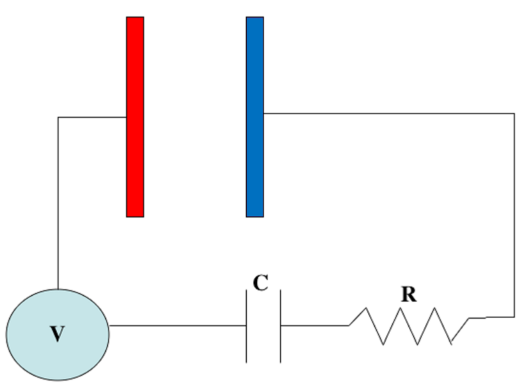

(c)

FIG. 1. Schematic diagrams of (a) a thermionic energy converter with an external load and (b) virtual cathode formation, and (c) OOPD1 model of a diode TEC with an external circuit.

performance. Some researchers had investigated the performance of solar powered TECs using the theory of finite-time thermodynamics and studied the characteristics of the system in the maximum power operation regime.[6] On the other hand, others have addressed the computer simulation of plasmas using a particle-in-cell (PIC) approach, and this approach is a convenient way to study the TEC problem.[7,8] In this work, we describe the development, verification, and ongoing extension of a one-dimensional numerical model for analyzing the TEC performance more precisely with less computing resource using a bounded finite-difference time-domain (FDTD) PIC plasma simulation code, OOPD1 developed formerly by the Plasma Theory and Simulation Group (PTSG), formerly at UC Berkeley[9] and now at Michigan State University. We have verified the feasibility of studying and developing TECs via numerical simulations by first benchmarking the OOPD1 simulation results with some analytical calculations.

II. MODELING THE THERMIONIC ENERGY CONVERTER

A TEC is formed by two parallel electrodes, the emitter and the collector. The emitter is heated, causing electrons to be thermionically emitted with a Maxwellian flux. Electrons cross the gap between the plates and are collected at the collector. If the collector has a higher Fermi potential than the emitter, the electrons will have a net potential gain equal to the difference in Fermi potentials. For a simple diode configuration, as modeled in this initial work, the electrons are emitted at the Fermi potential of the emitter, and collected at the Fermi potential of the collector plus the gap voltage and the output load voltage. The difference in potential can be used to perform electrical work. In the following, we introduce the analytical model to describe and understand the basic working mechanisms of a TEC and which also serves as a benchmark standard for our study on the feasibility of modeling a TEC using particle-in-cell simulations. The objective of this study is to establish a diode-based TEC numerical model by using a bounded FDTD PIC numerical method. The TEC model can be the basis for the development of a modified triode TEC for improving energy conversion efficiency and practicality of the TEC.

A. Analytical model

TECs are based on thermionic emission, a process where electrons are emitted from a high temperature metal or metal-oxide surface. The current emitted is governed by the Richardson-Dushman equation[10,11]

$$J_{RD} = AT^2 \exp\left(-\frac{\phi}{kT}\right), \tag{1}$$

where A is the Richardson-Dushman constant, φ is the work function of the material, T is the temperature of the surface, and k is the Boltzmann's constant. From the Carnot efficiency, the upper bound on energy performance of a TEC is proportional to the temperature difference between the emitter and the collector. If the temperature difference is high enough, for example, 1800 °C, the energy efficiency will be above 80%. But the real problem is the TEC performance will be restricted by the space charge limit. Consider a one-dimensional TEC model with an external load, as shown in Fig. 1(a). The emitter and the collector are infinite parallel planes, the space charge limited current is determined by Child-Langmuir Law[4,5]

$$J_{CL} = \frac{4}{9}\varepsilon_0\sqrt{\frac{2e}{m}}\frac{V^{3/2}}{d^2}, \tag{2}$$

where V is the voltage across the gap of the emitter and the collector, e is the electron charge, m is the electron mass, ε_0

is the permittivity of vacuum, and d is the length of the gap. The Child-Langmuir law can be extended to account for initial averaged velocity for emitted electrons[12,13]

$$J_{CL,v_0} = \frac{4\varepsilon_0}{9d^2}\sqrt{\frac{2e}{m}}\left(\sqrt{V+\frac{mv_0^2}{2e}}+\sqrt{\frac{mv_0^2}{2e}}\right)^3. \tag{3}$$

In this case, although more transmitted current can be expected, a virtual cathode or a potential barrier will be formed around cathode surface, as shown in Fig. 1(b), due to the increased space charges of electrons. Obviously, the key to increase the efficiency of TECs is to find the ways to increase the space charge limit. In order to verify the accuracy of the TEC numerical model, we have benchmarked the extended Child-Langmuir law, i.e., Eq. (3).

To treat the thermal effect more carefully, consider the emitted electrons as a Maxwellian flux distribution. We employ the numerically exact solutions developed by Langmuir[14] to get the maximum transmitted current and the corresponding potential distribution in the inter-electrode gap of a TEC. The numerically integrable formula is expressed as

$$\xi = \int_0^\eta \frac{d\eta}{\left(e^\eta - 1 \pm e^\eta erf\left(\sqrt{\eta}\right) \mp 2\sqrt{\eta/\pi}\right)^{1/2}}, \tag{4}$$

defining two dimensionless variables

$$\eta = e(\varphi - \varphi_m)/kT, \tag{5}$$

$$\xi = 4\left(\frac{\pi}{2kT}\right)^{3/4} m^{1/4}\sqrt{eI}(x - x_m). \tag{6}$$

Here, $\pm$ is determined by the positive and negative of "$x - x_m$." This integral can be evaluated numerically using the Standard Quadratic Method.[2] Therefore, we can obtain the *J*-*V* curve and *w*-*V* curve of the 1-D TEC model through the theory.

B. Particle-in-cell model

We have constructed a diode-based TEC model in the OOPD1 code.[15] OOPD1 is an object-oriented 1-D electrostatic particle-in-cell plasma simulation program. It solves the equations of motion for particles in continuum space and the Poisson equation on a discrete spatial mesh. Linear interpolation is used to obtain the source term for Poisson's equation on the discrete mesh, and linear interpolation is also used to obtain the electric field at the continuum particle locations from the discrete mesh.[9] The numerical model established in this study contains an external circuit, as shown in Fig. 1(c). The boundary conditions of the electric field and particle emission, and absorbing boundary conditions in the numerical model are assigned appropriately to represent the operation of a TEC. The system considered is the same as that in the analytical model, with the addition of an external circuit. In order to compare to the analytic model which lacks an external circuit, initially we set $R = 0$ and $C = 5$ F, effectively shorting the circuit. For the initial model, we consider only electrons, without a background gas and plasma generation.

The hot thermionic cathode is modeled by specifying a fixed emitted electron current, J_{RD}, representing the Richardson-Dushman thermionic current at a fixed temperature. The mean velocity of emitted electrons is $\overline{v_0} = v_{te1} = (kT/m)^{1/2}$ (Ref. 14) or $\overline{v_0} = v_{te2} = (\pi kT/2m)^{1/2}$,[16] since the model is 1-D. The final parameter is the voltage across the gap. Here, there is a subtlety, since in the literature the voltages are defined slightly differently. In the literature, the electrode output voltage V is defined as

$$V = \mu_C - \mu_E, \tag{7}$$

where μ_E and μ_C are the Fermi energies of the emitter and collector, respectively. μ_E is usually taken to be the ground energy in the system. The output voltage is the net potential an electron would gain in traversing the gap. However, in OOPD1, voltage is defined as the unloaded voltage across the gap, which is not equal to V. The voltage across the gap is actually

$$\begin{aligned} V_{OOPD1} &= (\phi_E + \mu_E) - (\phi_C + \mu_C) \\ &= \phi_E - \phi_C - V \\ &= V_0 - V, \end{aligned} \tag{8}$$

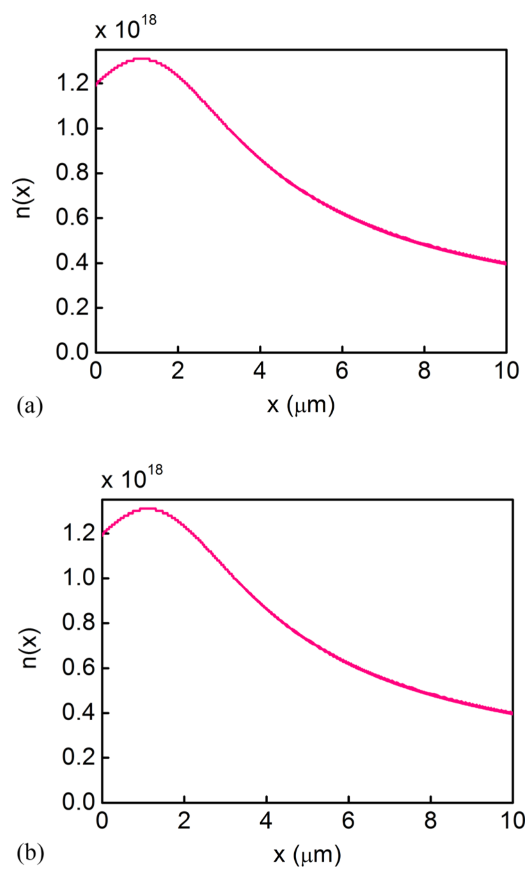

FIG. 2. (a) Electron distribution along the gap and (b) phase space ($x - v_x$) of the OOPD1 diode model with a gap distance of 10 μm, an applied voltage $V = 0.6$ V, and an injected current density equal to 36 200 A/m^2 (under the space charge limit) with an average initial velocity $v_0 = 188\,984$ m/s.

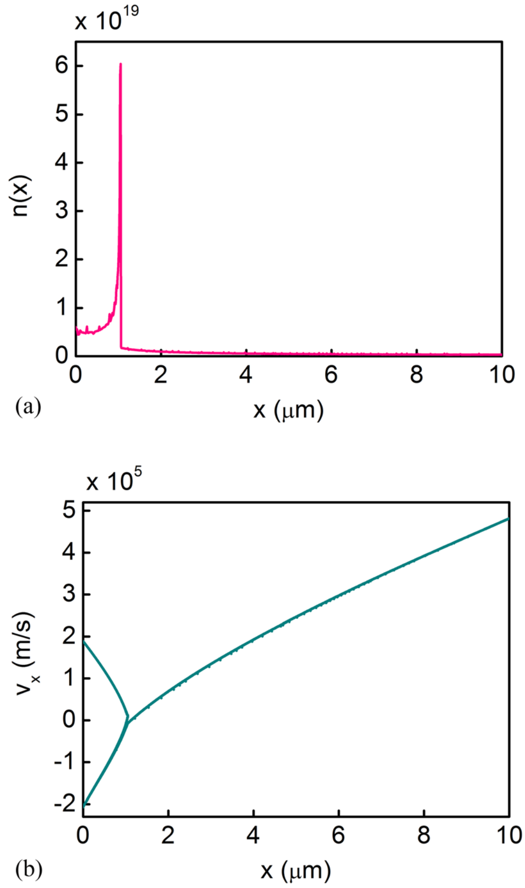

FIG. 3. (a) Electron distribution along the gap and (b) phase space $(x - v_x)$ of the OOPD1 diode model with a gap distance of 10 μm, an applied voltage $V = 0.6$ V, and an injected current density equal to 40 000 A/m^2 (over the space charge limit) with an average initial velocity $v_0 = 188\,984$ m/s.

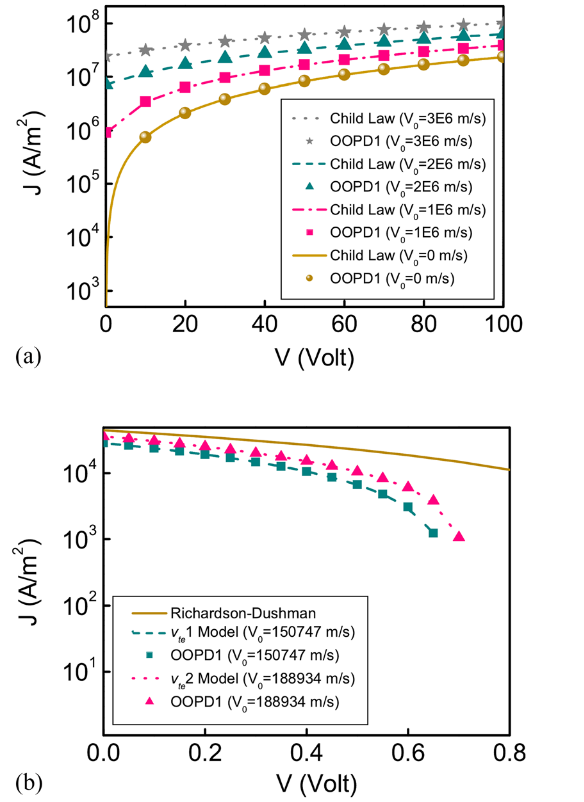

FIG. 4. OOPD1 simulation results of current density versus voltage (*J-V*) curves for a planar diode with (a) higher voltages and (b) lower voltages (TEC operating regime) indicated by the symbols are compared with the analytical results of the Child-Langmuir diode, represented by the lines showing good agreement.

where V_0 is the contact potential, and ϕ_E and ϕ_C are the work functions of the emitter and collector, respectively. Thus, to simulate a certain electrode output voltage V in OOPD1, we must use the work functions to calculate the voltage across the gap. Using this voltage and the settings given above, we can calculate the *J-V* and *w-V* curves. The simulation results are further compared with the analytical model to verify the accuracy of the TEC simulation model.

III. SIMULATION RESULTS AND DISCUSSION

We have verified the feasibility of studying and developing TECs via numerical simulations by first benchmarking the OOPD1 simulation results with the analytical calculations mentioned above. In the OOPD1 simulations of a Child-Langmuir diode, the current emission is set to be a constant value and the space charge limit, i.e., the maximum current transmitted across the gap, is measured by varying the injected current until a virtual cathode oscillation forms. For example, when we set $V = 0.6$ V and the injected current density from the cathode on the left-hand side equal to 36 200 A/m^2, just under the space charge limit with a gap distance of 10 μm and an initial velocity of $v_{te2} = 188\,934$ m/s, the electron distribution in the gap is smooth and the electron current is totally transmitted across the gap, reaching the anode on the right-hand side, as shown in Fig. 2. Increasing the injected current density to 40 000 A/m^2, a little larger than the space charge limit, a virtual cathode is quickly formed near the emitter and some electrons get reflected back to the cathode by the virtual cathode potential barrier, as shown in Fig. 3. Figure 4(a) shows the simulation results of the OOPD1 model of a planar diode with a gap distance of 10 μm under higher applied voltages up to 100 V, in good agreement with the analytic results of the Child-Langmuir law (zero initial velocity) and its extension with an injection velocity of 1×10^6, 2×10^6, and 3×10^6 m/s. Similarly, Figure 4(b) shows the simulation results of the same OOPD1 diode model but for lower voltages, i.e., the operating regime of a TEC, with an average initial velocity of $v_{te1} = 150\,747$ m/s and $v_{te2} = 188\,394$ m/s for the injected electrons corresponding to an emitter temperature of 1500 K, also in good agreement with the analytical prediction.

To further consider the thermal effect in a TEC more carefully, with the electrons emitted from the cathode in a Maxwellian flux distribution, the numerically exact solutions developed by Langmuir mentioned above gives an idealized current-voltage profile. However, since OOPD1 simulates the same system that the analytic model treats (with the input file configured appropriately), OOPD1 should reproduce the *J-V* and *w-V* curves. To test this, steady-state currents for several output voltages have been measured and compared to

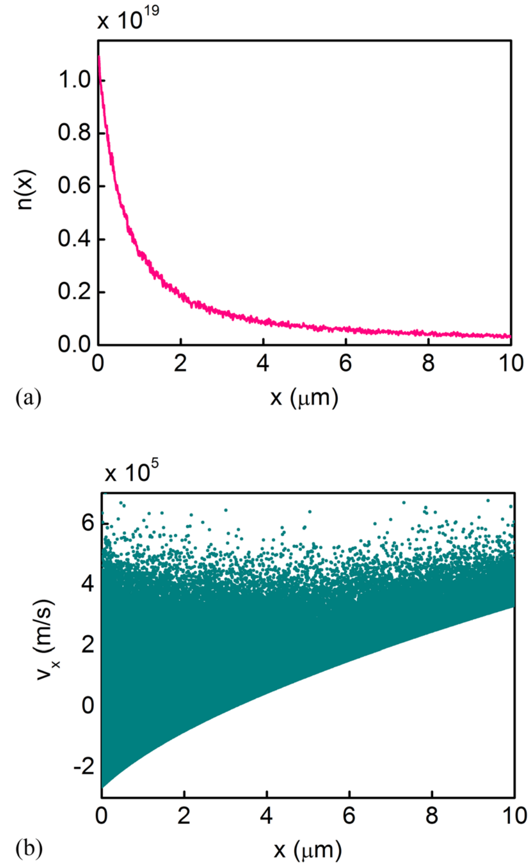

FIG. 5. (a) Electron distribution along the gap and (b) phase space ($x - v_x$) of the OOPD1 TEC model with a gap distance of 10 μm, an applied voltage $V = 0.3$ V, a current density emitted according to the Richardson-Dushman law, Eq. (1). Here, the injected electrons are assigned with initial thermal velocities of a Maxwellian flux distribution, corresponding to an emitter temperature of 1500 K.

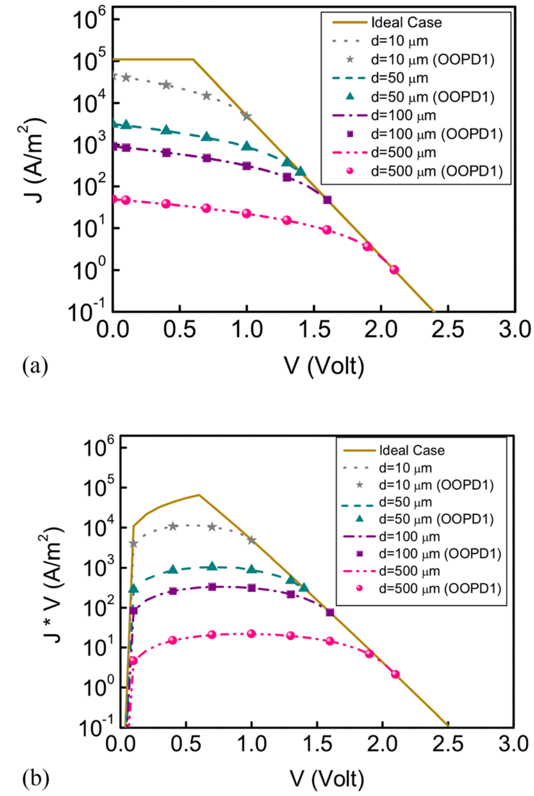

FIG. 6. OOPD1 simulation results of (a) current density versus voltage (J-V) curves and (b) power flux density versus voltage (w-V) curves indicated by the symbols are compared with the results of the analytical model represented by the solid lines, showing good agreement.

the theoretical results. Figure 5 shows the emitted charge distribution across the gap and the phase space information from the OOPD1 simulation of a TEC model with a gap distance of 10 μm, $V_{OOPD1} = 0.3$ V, i.e., an output voltage of 0.3 V for an emitter and collector work functions of 2.2 eV and 1.6 eV, respectively, and a current density emitted according to the Richardson-Dushman law, Eq. (1). Here, the injected electrons are assigned with initial thermal velocities of a Maxwellian flux distribution,[17] corresponding to an emitter temperature of 1500 K. One can see from Fig. 5(b), interestingly, electrons are spread in velocity and a large portion of slow electrons are reflected back to the cathode due to the space charge effects of electrons near the turning point.

For TECs of gap widths in the range from 10 to 500 μm, the current density-voltage (J-V) characteristic curves and the power flux density-voltage (w-V) curves from OOPD1 simulations are shown in Figure 6. The simulation results for all the gaps indicated by symbols show excellent agreement with the analytic results which are shown with lines. Therefore, OOPD1 reproduces the theoretical results very closely in the limit of the idealized conditions of the theory, indicating that the code is working correctly. The effects of space charge are clear from Fig. 6. The right- and top-most solid line noted as "ideal case" on the plots is called the Boltzmann line, and gives the current and output power densities in the absence of space charge effects, the ideal case. Clearly, as the gap spacing increases the current falls far short of the Boltzmann line, indicating suboptimal performance. From Fig. 6(b), the output power is reduced by several orders of magnitude for large gap spacing. Much research has gone into determining how to effectively fabricate extremely small gaps (on the order of 10 μm) in an effort to increase the output power, but maintaining uniform gap spacing remains difficult and expensive. Our eventual goal is to model the TEC proposed in Ref. 3, in order to study mitigation of the negative space charge by ions. As the new design (and almost all existing TECs) use positive cesium ions to neutralize space charge, our immediate work will be on adding a cesium collision model. The primary difficulty encountered so far is ensuring that the cesium ionization process is modeled accurately. As cesium has many electrons, there are a large number of excited states, meaning that multi-step ionization plays an important role in ion production. Finding accurate cross-sections for these reactions has proved difficult. In addition, OOPD1 will need to be modified to track metastable states.

IV. CONCLUSION

The feasibility of simulating a thermionic energy converter using a bounded finite-difference time-domain particle-in-cell plasma simulation code, OOPD1, developed by PTSG, formerly at UC Berkeley and now at Michigan State University, has been studied. We have successfully used OOPD1 to model a TEC kinetically for the first time and verified its accuracy for an analytically solvable case. The general expressions for TEC behaviors are revisited. Through the preliminary numerical results, it is found that: (1) the simulation results of the OOPD1 TEC model are in good agreement with the analytical predictions and (2) the maximum transmitted current through a TEC limited by space charge effects can be obtained. These preliminary results encourage us to use particle-in-cell simulations for the optimal design and study of practical TECs. In our future work, a more advanced scheme is a triode configuration used to confine fast electrons in order to generate ions to increase the space charge limit in the gap. TECs are fascinating devices that have the potential to substantially increase in efficiency. With OOPD1, we will be able to quickly and cheaply analyze space charge effects, and seek designs that mitigate the space charge effect, enabling TECs to become more efficient and cost-effective. The advantage of the PIC code is that it makes no assumptions about the external circuit state, charged particle profiles and distribution functions, and allows these to evolve self-consistently.

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